## THE PLTEMP V2.1 CODE

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### **ABSTRACT**

Recent improvements to the computer code PLTEMP/ANL V2.1 are described. A new iterative, error-minimization solution technique is used to obtain the thermal distribution both within each fuel plate, and along the axial length of each coolant channel. A new, radial geometry solution is available for tube-type fuel assemblies. Software comparisons of these and other new models are described. Applications to Russian-designed IRT-type research reactors are described.

### Introduction

PLTEMP/ANL V2.1 is a FORTRAN program that obtains a steady-state flow and temperature solution for a nuclear reactor core, or for a single fuel assembly. It is based on an evolutionary sequence of "PLTEMP" codes in use at ANL for the past 20 years [1-7]. Fueled and non-fueled regions are modeled. Each fuel assembly consists of one or more "elements" (plates or tubes) separated by coolant channels. The temperature solution is effectively 2-dimensional. It begins with a 1-dimensional solution across the fuel elements within a given fuel assembly, at the entrance to the assembly. The temperature solution is repeated for each axial node along the length of the coolant channel. The geometry may be either slab or radial, corresponding to fuel assemblies made from a series of flat (or slightly curved) plates, or from nested tubes. A variety of thermal-hydraulic correlations are available with which to determine safety margins such as onset of nucleate boiling (ONB), departure from nucleate boiling (DNB), and onset of flow instability (FI). Coolant properties for either light or heavy water are obtained from FORTRAN functions rather than from tables. The code is intended for thermal-hydraulic analysis of research reactor performance in the sub-cooled boiling regime.

### User options and models

The coolant mass flow rate by channel may be input directly. Margins to DNB and to FI based on outlet coolant temperature values are calculated. Given an axial relative power distribution, the code computes the heat flux profile and corresponding temperatures for the fuel, clad and coolant. Nodes in sub-cooled nucleate boiling and fully-developed nucleate boiling based on either the Bergles-Rohsenow [8] or the Forster-Greif [9] correlation and the Jens-Lottes [10] correlation, respectively, are flagged in the output. The power at ONB can be determined manually. A series of calculations can be performed in one run to span a desired range of powers or pressure drops.

The fuel element dimensions are specified by the width or arc length of the fuel meat and the unfueled portion, if any. This gives the user the freedom to describe flat plates or curved plates of varying size such as concentric cylinders of fuel with no unfueled region. If plate radii are large compared with the thickness of the plate, the plate geometry solution is still a good approximation for curved plates or cylinders. The solution allows a choice of single-phase heat transfer coefficient that include the Sieder-Tate [11], Dittus-Boelter [12] and Colburn [13] correlations. The Critical Heat Flux (CHF) options include the Mirshak-Durant-Towell [14], Bernath [15], Labuntsov [16] and Mishima [17] correlations for Departure from Nucleate Boiling (DNB) and the Whittle-Forgan correlation for Flow Instability (FI) [18]. The Jens-Lottes [10] correlation is imposed for two-phase heat transfer, and the Bergles-Rohsenow [8] or the Forster-Greif [9] correlations are used to detect the Onset of Nucleate Boiling (ONB). Also available are the Mishima [17] and Weatherhead [19] CHF correlations, and two Russian heat transfer correlations: Petukhov [20] and a slightly modified Dittus-Boelter correlation of the form Nu = 0.021 Re<sup>0.8</sup> Pr <sup>0.43</sup> (Pr/Pr<sub>w</sub>) <sup>0.25</sup>.

### Description of error-minimization solution to fuel plate temperature profile

The procedure used in earlier versions of PLTEMP estimated the location of the peak fuel temperature within a given plate from channel-average heat fluxes on either side. This process was inconsistent in that the peak fuel temperature within a given plate could be predicted from each side, but the location and value of the peak fuel temperature was not corrected to eliminate the mismatch. PLTEMP/ANL V2.1 replaced the procedure used in earlier versions of PLTEMP with a new iterative procedure to find the location and value of the peak temperature in the fuel. This location influences every other predicted temperature and heat flux. The solution process is now totally iterative, assuming conditions for the coolant entering a particular axial node are known and that the heat production rate within the node is also known. First, the standard PLTEMP solution is obtained, and used as a basis for iterative refinement. A globally convergent technique known as Broyden's Method [21] is used to solve the equation  $\mathbf{F}(\mathbf{x}) = 0$ , where F is a vector of peak fuel element temperature differences as obtained from either side and  $\mathbf{x}$  is the solution vector containing the fractional position of the peak temperature in each plate. This method numerically determines the Jacobian matrix of partial derivatives that is needed to refine the vector x. The solution proceeds iteratively until the peak fuel temperature differences are all less than a specified tolerance (typically results are good to less than 0.01 degree). While this process is ongoing, all heat transfer coefficients, coolant temperatures, clad temperatures, and fuel temperatures are continuously updated. The final temperature solution is therefore completely self-consistent.

## **Radial geometry solution**

Another extension to PLTEMP capabilities is an option that permits curved plates or annular fuel tubes (with similar channels). The temperature profile can now be obtained at user option in either slab or radial geometry. Since fuel and clad thicknesses are the same for all plates of a given fuel assembly type, it is only necessary to provide the radius of curvature for the centerline of each plate or tube. The mathematical equations solved are changed to account for curvature, as are the heat fluxes. The code detects the sequence of the plates: from the largest to the

smallest radius of curvature, or vice-versa. Internal logic and equations permit the user to specify the problem in either orientation.

In one-dimension radial geometry, the heat conduction equation can be written:

$$d^2t/dr^2 + (k/r)dt/dr + q''' = 0$$

where k is the thermal conductivity of the medium and q'' is the volumetric heat source strength. The solution is

$$t = -q$$
"  $r^2/(4k) + C_1 \ln[r] + C_2$ 

At the point of maximum temperature,  $r_m$ , the derivative of temperature with radius is zero:

$$dt/dr = -q^{"} r/(2k) + C_1/r \rightarrow 0$$

The solution is  $C_1 = q^{"} r_m^2/(2k)$ . Assuming that the temperature is  $t_{out}$  at the outside (largest radius of curvature) of the fuel plate, then

$$t_m - t_{out} = q''' / (2k) \{ (r_{out}^2 - r_m^2)/2 - r_m^2 \ln[r_{out}/r_m] \}$$

Similarly, assuming that the temperature is t<sub>in</sub> at the inside (smallest radius of curvature) of the fuel plate, then

$$t_m - t_{in} = q^{"}/(2k)\{-(r_m^2 - r_{in}^2)/2 + r_m^2 ln[r_m/r_{in}]\}$$

We want to know the fraction of the heat  $Q = q^{"}V$  generated on each side of the maximum temperature point, for use in the overall temperature solution. The fraction "on the left," outside the annulus, is obtained for an assumed flat q''' profile across the fuel meat annulus from  $x = Q_1/Q = (r_{out}^2 - r_m^2)/(r_{out}^2 - r_{in}^2) = (r_{out} + r_m)(r_{out} - r_m)/(2r_{mid}\delta)$ 

$$x = Q_1/Q = (r_{out}^2 - r_m^2)/(r_{out}^2 - r_{in}^2) = (r_{out} + r_m)(r_{out} - r_m)/(2r_{mid}\delta)$$

In this equation,  $\delta$  is the fuel meat thickness, and  $r_m = r_{out} \sqrt{1 - 2 r_{mid} \delta x / r_{out}^2}$ .

For the temperature drop across the clad of thickness  $\varepsilon$ , let the following radii be defined:

 $r_1 = r_{mid} + \delta/2 + \epsilon$ ;  $r_2 = r_{mid} + \delta/2$ ;  $r_3 = r_{mid} - \delta/2$ ;  $r_4 = r_{mid} - \delta/2 - \epsilon$ . Then it is necessary to determine clad effective thickness terms of the form:  $r_1 \ln[r_1/(r_1 - \varepsilon)]$ ;  $r_4 \ln[(r_4 + \varepsilon)/r_4]$ . The temperature drop across the clad on the left or right, given heat flux  $J_1$  or  $J_2$  becomes:

$$t_2 - t_1 = r_1 \ln[r_1/(r_i - \varepsilon)] J_1/k_{clad}$$
  
 $t_4 - t_3 = r_4 \ln[(r_4 + \varepsilon)/r_4] J_r/k_{clad}$ 

For comparison, the temperature drop across the clad, in slab geometry, given heat flux J is:

$$t_2 - t_1 = J \varepsilon / k_{elad}$$

# Friction factors for smooth pipes and rough pipes

For turbulent flow, friction factors for sections of reactor fuel assemblies and bypass channels can be obtained from  $f = A(Re)^{-B}$ , given A and B from experiment. Coefficients A and B together account for surface roughness and actual geometry. If no such fitted data exists, PLTEMP/ANLV2.1 now will obtain default friction factors f appropriate to hydraulically smooth pipes following Moody [22]. The equation for the Fanning friction factor f' at Reynolds number Re satisfies:

$$1/\sqrt{f'} = 4.* \text{Log}_{10}[\text{Re } \sqrt{f'}] - 0.4$$

*Mathematica* was used to solve this expression for f':

$$f' = 6.25002/(1. - 8.68591 \text{ Log}_e[\text{Re } \sqrt{f'}] + 18.8612 (\text{Log}_e[\text{Re } \sqrt{f'}])^2)$$

This expression for f' can easily be solved recursively starting with a trial value of f', typically in less than 10 recursions, for relative error  $\leq 1.0 \times 10^{-5}$ . Then the Darcy-Weisbach friction factor f = 4f', as given by Moody, follows directly.

For rough pipes, the user supplies the relative surface roughness  $e/D_e$  as a parameter ( $0 \le ROUGH(I) \le 0.1$ ). This f' is solved iteratively using the smooth pipe result as a starting guess.

$$f'=0.331369/Log_e[0.27027e/D_e + 1.255/(Re \sqrt{f'})]^2$$

Then the Darcy-Weisbach friction factor f = 4f', as given by Moody, follows directly.

### **Software verification**

A computation of energy out from all coolant channels was added in order to confirm the energy balance: heat out = heat in. At user option, the fluid specific heat and density can be fixed for the run. This has been of some assistance when comparing results with those from other codes that only have this option. *Mathematica* was used to determine the correct equations to use for radial geometry. It was also used to perform verification of some specific temperature profiles. For example, calculations were performed for variations on the IAEA Generic 10 MW Reactor [23] to check the peak fuel temperature from the code vs. results from *Mathematica*. A single axial node model was used for this check. The general solution for the peak fuel temperature in slab geometry with flat heat source volumetric strength s, conductivity k, thickness d, and boundary temperatures t1 and t2 (in *Mathematica* notation) is:

pf[t1\_,t2\_,k\_,s\_,d\_]:={
$$4k^2(t_1 - t_2)^2/d^2 + (4 k s)(t_1 + t_2) + s^2d^2$$
}/(8 k s)  
The location of the peak fuel temperature is:  
 $x \rightarrow (2 k t_1 - 2 k t_2 + s x_1^2 - s x_2^2)/(2s(x_1 - x_2))$ .

Table 1. Check of peak fuel temperature in slab geometry

Power, MW	Clad/Fuel Temp., C	Peak Fuel Temp., C PLTEMP/ANL V2.1	Peak Fuel Temp., C Mathematica
0.01	69.9454	103.014	103.014
0.02	89.5427	155.680	155.690
0.03	108.8295	208.036	208.036

In radial geometry, with flat heat source volumetric strength s, conductivity k, x1 and x2 the radii of the two exterior surfaces with boundary temperatures t1 and t2, the general solution for the peak fuel temperature (in *Mathematica* notation) is:

$$\begin{split} r[t1\_,t2\_,k\_,s\_,x1\_,x2\_] &:= \\ \{2(4k\ t2+s\ x2^2)Log[x1]-2\ (4k\ t1+s\ x1^2)Log[x2]+ \\ (4k\ (t1-t2)+s(x1^2-x2^2)) \\ \{-1+2\ Log[-\ C1/C2])\}\}/(8k(Log[x1/x2]));\ C1=\sqrt{\{4k(t2-t1)+s(x2^2-x1^2)\}} \\ C2&=\sqrt{\{2s\ Log[x2/x1]\}} \end{split}$$

The location of the peak fuel temperature is:

$$x \rightarrow \sqrt{\frac{4k[t_2 - t_1] + s[x_2^2 - x_1^2]}{\sqrt{2s(Log[x_2] - Log[x_1]}}}$$

The computed hydraulic solution for unheated pipe flow was validated against analytical solutions for mass flow rate. Simple networks of parallel pipes were also validated.

### Validation of Whittle & Forgan flow instability

Auxiliary calculations were made of the onset of flow instability from the Thermal-Hydraulic Test Loop (THTL) of ORNL experiments [24]. Cases FE714B (5.3 MW/m<sup>2</sup>) and FE105D (14.92 MW/m<sup>2</sup>) were modeled as a single heated plate. The heat flux at Onset of Flow Instability (OFI) was predicted by PLTEMP/ANL V2.1 within 2% of the linear fit [24] of:

 $M_{ofi}$  (1000 kg/m<sup>2</sup>s) = 1.455 q, where q is the average heat flux in MW/m<sup>2</sup>.

### **Engineering hot-channel factors**

Historically, engineering hot channel factors (HCF) have been used to estimate the safety implications of deviations from fuel and core design specifications that are caused by either random effects or by specific physical effects.  $F_b$  is the HCF for the global bulk coolant temperature rise.  $F_h$  is the HCF for the heat transfer coefficient to the coolant.  $F_q$  is the hot channel factor for heat flux from the meat. The PLTEMP/ANL V2.1 code permits the user to use any or all of  $F_q$ ,  $F_b$ , and  $F_h$ . But the solution technique is new. In the event that hot channel factors differing from unity are provided, the base case conditions are solved without HCF's. Second, the HCF's are applied to the base condition solution, without alteration of the location of the peak fuel temperature points. Third, the HCF's are applied to the base condition solution, with a full solution permitting everything to vary in order to reach the new steady-state solution. All three problem conditions are solved in a single run.

In PLTEMP/ANL V1.0,  $F_q$  was applied to either side of a fuel plate meat when calculating the heat flux moving left and right. The ratio of heat fluxes was used to estimate the location of the peak fuel temperature point from:

$$\delta = t_{\text{meat}}/(1. + Q_{\text{r}}/Q_{\text{l}})$$

Consequently, the width of the fuel meat section to which  $F_q$  was applied varied with the problem. For ease of understanding, the methodology is now changed to assure that  $F_q$  is applied to either the left or right half of the fuel meat. In that event, it is clear that the location of the peak fuel temperature should be shifted from plate center toward the side with higher power.

Consider the problem of solving for the temperature profile for the excess heat produced by  $F_q$  >1. Assume that the excess heat is on the left half of the fuel meat. In slab geometry, the heat fluxes will be:

$$Q1 = (F_q - 1)s x_{max} A$$

where s is the normal volumetric heat source strength (J/s/m<sup>3</sup>), A is the heat transfer area (m<sup>2</sup>), t is the fuel meat thickness, and  $0 \le x_{max} \le t/2$ . Assuming that the fuel temperature is  $t_1$  on the left surface of the meat and  $t_3$  on the right, and  $t_m$  at the maximum, then:

$$t_m - t_3 = \{ (F_q - 1)s/(2 k_f) \} \{ 3t^2/4 - 2 x_{max} d + x_{max}^2 \}$$

If we define the nondimensional location  $X = x_{max}/t$ , then

$$t_m - t_3 = \{(F_q - 1)s t^2/(2 k_f)\}\{3/4 - 2 X + X^2\}, \text{ for } 0 \le X \le \frac{1}{2}.$$

For  $X > \frac{1}{2}$ , all of the excess heat from  $(F_q - 1)$  flows to the left (recall that it exists only for  $X \le \frac{1}{2}$ ). In that case, the contribution to  $t_m$  -  $t_3$  is zero. Here  $k_f$  is the meat thermal conductivity. On the left hand side.

$$t_m$$
 -  $t_1$  = {(f-1)s  $t^2/(2 k_f)$ } { $X^2$ }, for  $0 \le X \le \frac{1}{2}$ .

By substituting Y=1-X, one obtains the symmetrical equations for  $F_q$  applied on the right.

# Limits of operation

Whole-core modeling capabilities are now greatly expanded. There may be up to 60 different types of fuel assemblies (up to 30 of each), and up to 50 different types of bypass channels (up to 50 of each). Older versions of the code were limited to 5 different types of fuel assemblies and 5 different types of bypasses. Light water properties extend to 340 C.

## Thermal-hydraulic safety analysis for IRT-3M and IRT-4M fuel in the WWR-CM reactor

The work reported is for IRT-4M fuel assemblies with operating conditions and dimensions specified in Refs. [25-26]. For comparison with these calculations, the coolant specific heat was fixed at 4180 J/kg/C and the density was fixed at 1000 kg/m<sup>3</sup>. The heat transfer correlation used was a slightly modified Dittus-Boelter correlation of the form:

$$Nu = 0.021 \text{ Re}^{0.8} \text{ Pr}^{0.43} (\text{Pr/Pr}_w)^{0.25}$$

A slightly modified Forster-Greif boiling correlation was used:

$$\Delta T_{sat} = 2.04 \text{ q}^{-0.35} / P^{0.25}$$
, where  $T_w = T_{sat} + \Delta T_{sat}$ .

Here q is the heat flux  $(kW/m^2)$ , and  $P_c$  is the pressure of the coolant (bar). The Labuntsov correlation was used for Critical Heat Flux:

$$q_c = 1.454 \theta(P)[1+2.5U^2/\theta(P)]^{1/4} \times [1 + 15.1 \text{ Cp } \Delta T_{\text{sub}}/(\lambda P^{1/2})],$$

Here  $\theta(P) = 0.99531 \text{ P}^{1/3} (1 - P/P_c)^{4/3}$ ,  $\lambda$  is the latent heat of vaporization (kJ/kg),  $C_p$  is the specific heat of the coolant (kJ/kg/K), and  $P_c$  is the critical pressure of the coolant (bar).

IRT-3M or IRT-4M fuel assemblies (nested square tubes with rounded corners) can be modeled as equivalent inscribed cylinders. We are interested in how different modeling assumptions compare at predicting operating conditions in these fuel assemblies. PLTEMP/ANL V2.1 solves for thermal-hydraulic conditions in either slab or cylindrical geometry. As such, it can model the fuel in two approximations to the actual 3-dimensional geometry. Since most of the heated area of the fuel plates is flat, and the radius of curvature is relatively large compared to the plate thickness, one should expect that the slab approximation will be best. Use of an equivalent set of nested cylinders in radial geometry will provide some sense of the error introduced in calculations by being forced to use an approximate geometrical model. The results shown in the tables between slab and radial geometry solutions are very consistent.

#### Fuel assembly models

Problem 1 represents a 6-tube low-enriched uranium (LEU, 19.7%) IRT-4M fuel assembly. Cases C1 and C1r are geometrically created by choosing cylindrical tubes with outer diameters equal to the flat-to-flat o.d. of each square tube. The first coolant channel diameter is based on an outer radius equal to the fuel assembly pitch. It therefore is a "half-channel," because of the plane of symmetry between fuel assemblies. This model is good for approximating conditions near the middle of the flat sides of the actual fuel assembly. Cases C3 and C3r account for all of the water in the actual fuel assembly coolant channels. This model therefore represents average conditions. It should not be as conservative as the model used in cases C1 and C1r.

Temperatures were calculated at 11 nodal interfaces, with all nodes 0.1 relative unit in length. PLTEMP/ANL V2.1 calculates temperatures at nodal midpoints, as well as at the last interface for the coolant. Calculations were performed with PLTEMP/ANL V2.1 using the option to fix the coolant density and specific heat at 1000 kg/m<sup>3</sup> and 4180 J/kg-K, respectively.

## Modeling of assembly in slab geometry

First, the coolant mass flow rates are revised to match the channel velocities. Then the power is adjusted to match the desired peak power density. PLTEMP/ANL V2.1 used the "Russian" correlation for generating heat transfer coefficients. For the present cases, the Reynolds numbers exceed 10000. We used the Forster-Greif boiling correlation (for ONB). The Labuntsov CHF correlation indicator is also used by PLTEMP/ANL V2.1 for DNB.

#### **Conclusions**

Results are given in tables 2 and 3, which give results from four variations of the problem.

- 1. The cylindrical geometry option affects calculated peak fuel temperatures slightly, particularly for the plate with the smallest radius of curvature.
- 2. Coolant exit temperatures agree typically within 0.5 degree. The flow is clearly stable. The presence of the extra water from the corners is particularly noticeable in channel 1, when comparing C1 vs. C3 or C1r vs. C3r.
- 3. The "inscribed tube" model of cases C1 and C1r has a smaller ONB margin than does the "actual geometry" model of cases C3 and C3r, as expected. It is more conservative and better represents limiting conditions near the center of the flats.
- 4. The axial nodalization is fairly coarse with only 11 nodes. A larger number of axial nodes could smooth out the axial power peak, and could perhaps lead to a slightly better prediction of fuel element performance.

Table 2. Comparison of key parameters: PLTEMP/ANL V2.1, 6-tube LEU IRT-4M fuel assembly

CASE	C1	C1r	C3	C3r
Geometry	Slab	Cyl.	Slab	Cyl.
Power, MW	0.41775	0.41775	0.50267	0.50267
Peak Power Density, MW/m³	1569	1569	1569	1569
Flow, kg/s	5.8808	5.8808	7.8330	7.8330
Fuel Heated Area, m <sup>2</sup>	1.1097	1.1097	1.33521	1.33521
Velocity in Channel 1, m/s	3.04	3.04	3.04	3.04
Plate 1 power fraction	0.22426	0.22426	0.22457	0.22457
Coolant ∆T, C	16.99	16.99	15.35	15.35
Peak Fuel Temperature, C	86.1	86.2	85.5	85.1
Min. ONB channel/node	1.922	1.918	1.950	1.952
	2/8	2/8	2/8	2/8
Min. DNBR, Labuntsov	11.42	11.39	11.65	11.62
Min. eta'	246	245	253	253
Min. FIR, Whittle & Forgan	2.727	2.722	2.928	2.929
N <sub>sub</sub> /N <sub>Zu</sub> *	5.46	5.44	5.92	5.91

<sup>\*</sup> If  $N_{sub}/N_{Zu}$  >1.36, flow is stable

Table 3. Coolant exit temperatures (C): 6-Tube LEU IRT-4M fuel assembly

CASE	C1	C1r	C3	C3r
Geometry	Slab	Cyl.	Slab	Cyl.
Chan. 1 T <sub>out</sub>	63.1	63.5	58.5	58.7
Chan. 2 T <sub>out</sub>	64.3	64.4	62.8	62.8
Chan. 3 T <sub>out</sub>	63.5	63.5	62.1	62.1
Chan. 4 T <sub>out</sub>	62.9	62.9	61.5	61.5
Chan. 5 T <sub>out</sub>	62.6	62.6	61.2	61.2
Chan. 6 T <sub>out</sub>	60.8	60.8	59.6	59.6
Chan. 7 T <sub>out</sub>	54.0	53.7	53.7	53.5

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